(corrected on 30.11.2021)

Ex5a

Exercise 6

1 Term symbols of multi-electron atoms

Under consideration of Hund's rules, the term symbols for a given multi-electron configuration are formally constructed via the LS- or jj-coupling scheme. In addition, the Pauli principle only allows states, for which two electrons don't share an identical set of quantum numbers – or more rigorously speaking: The total wave function of the system must be antisymmetric with respect to exchange of two identical electrons.

(a) Consider a carbon atom in ground state electron configuration C: $1s^2 2s^2 2p^2$. Write down all the formal term symbols ${}^{2S+1}L_J$ in the LS-coupling scheme for the valence subshell. Now fill the following table with the possible combinations $(m_{l_1}^{2m_{s1}}\, m_{l_2}^{2m_{s2}})$ (so e.g. $(1^+\ 0^-)$) and eliminate those cases, which are not allowed by the Pauli principle.

		m_S		
		$+1$	0	-1
	$+2$			
	$+1$			
m_L	0			
	-1			
	-2			

Using the table, systematically determine those term symbols $^{2S+1}L_J$ from your list, that are actually realised. Finally, identify the ground state.

For comparison, determine the possible term symbols for an excited state of the carbon atom with an electron configuration $1s^2 2s^2 2p^1 3s^1$ (Why is this much easier?).

(b) Write down the ground state electron configuration for a lead atom (Pb) and the corresponding formal term symbols $(j_1, j_2)_J$ in the jj-coupling scheme for the valence subshell. This time, use the Pauli exclusion principle in combination with the Clebsch-Gordan coefficients (e.g. from `http://pdg.lbl.gov/2002/clebrpp.pdf`) to decide, which terms are allowed. Look up the ground state in the NIST Atomic Spectra Database (see note below).

Note: You can check your results with the levels listed in the Atomic Spectra Database from the NIST (`https://physics.nist.gov/PhysRefData/ASD/levels_form.html`). The neutral atoms can be found by searching for e.g. ‘Pb I’.

2 Characteristic X-ray spectrum

Using a X-ray tube with a molybdenum (Mo) anode, the following features were identified in the recorded spectrum (neglecting any fine structure):

label	wavelength λ (in Å)
K_α	0.723574
K_β	0.635952
K_∞	0.6196481

Note: K_∞ denotes the K (absorption) edge, where the energy of the cathode electrons impinging on the anode surpasses the ionization energy of the K-shell electron.

(a) Determine the energy levels of the shells K, L, M (in eV).

(b) Calculate the minimum energy to excite a L transition.

(c) Estimate the screening parameter of the nuclear charge for an electron in the K and in the L shell.

(d) Besides the emission of X-ray photons, what other types (plural) of radiation can originate from the X-ray tube’s anode? Briefly explain the underlying effects.

3 The helium atom

We consider a simple Hamiltonian for the helium atom using $\vec{r}_1$ and $\vec{r}_2$ for the positions of the two electrons:

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_{ee}$$
$$\text{with } \hat{H}_i = -\frac{\hbar^2}{2m_e}\nabla_i^2 - \frac{Ze^2}{4\pi\varepsilon_0}\frac{1}{r_i} \text{ and } \hat{H}_{ee} = \frac{e^2}{4\pi\varepsilon_0}\frac{1}{|\vec{r}_1 - \vec{r}_2|}.$$

(a) Which known effects have been neglected in the Hamiltonian?

(b) Using the Hamiltonian given above, we want to estimate the energy of the helium ground state $1s^2$ in first-order perturbation theory.

1. Calculate the energy $E^0(1s^2)$ of the two-electron system without the electron-electron interaction (i.e. $\hat{H}_{ee} = 0$). This will be the energy of the 'unperturbed' ground state corresponding to the spatial wave function

   $$\psi = \psi_{100}(r_1)\psi_{100}(r_2)$$

   where ψ_{nlm} denotes the well known one-electron Schrödinger spatial wave functions in hydrogen.

2. For easier evaluation, we can rewrite the first-order energy correction as a sum of two terms E_{12} and E_{21}:

   $$\Delta E(1s^2) = \langle\psi|\frac{e^2}{4\pi\varepsilon_0}\frac{1}{|\vec{r}_1 - \vec{r}_2|}|\psi\rangle = E_{12} + E_{21}.$$

   The term E_{12} describes the electrostatic potential energy of the charge distribution $\rho(r_i) = -e|\psi_{100}(\vec{r}_i)|^2$ of electron e_2^- in the electrostatic potential $V_{12}(r_2)$ produced by e_1^- at radial distance r_2. Because the charge of e_1^- in the region $r_1 < r_2$ acts like a point charge

   $$Q_1(r_2) := \int_0^{r_2} \mathrm{d}r_1 \rho(r_1) 4\pi r_1^2$$

   at the origin, we can write

   $$V_{12}(r_2) = \int_0^{4\pi} \mathrm{d}\Omega \int_0^{r_2} \mathrm{d}r_1 r_1^2 \frac{e^2}{4\pi\varepsilon_0}\frac{1}{|\vec{r}_1 - \vec{r}_2|}\rho(r_1) = \frac{Q_1(r_2)}{4\pi\varepsilon_0 r_2}.$$

   An equivalent argument can be made for E_{21} with $1 \leftrightarrow 2$.

   Use this to calculate the energy correction $\Delta E(1s^2)$ and the estimated total energy of the ground state.

(c) Write down the spectroscopic term symbol for the ground state electronic configuration $1s^2$, as well as those for excited states with configuration $1s^1 2s^1$ and $1s^1 2p^1$.